Message

From: Jarabek, Annie [/O=EXCHANGELABS/OU=EXCHANGE ADMINISTRATIVE GROUP (FYDIBOHF23SPDLT)/CN=RECIPIENTS/CN=8B1DE54D48E1429C8129F6499211DBDB-JARABEK, ANNIE]
Sent: 8/18/2021 5:09:06 PM
To: Todd J. Stedeford, Ph.D., DABT®, ERT, ATS [TStedeford@lawbc.com]
Subject: RE: Can you tell me

Thank you. We have lost such a resource and font of wisdom with your departure.

From: Todd J. Stedeford, Ph.D., DABT®, ERT, ATS <TStedeford@lawbc.com>
Sent: Wednesday, August 18, 2021 12:48 PM
To: Jarabek, Annie <Jarabek.Annie@epa.gov>
Subject: RE: Can you tell me

Hi Annie,

All is good here, thanks. PMN folks use the analogue identification methodology (AIM). The public version is available at: https://www.epa.gov/tsca-screening-tools/analog-identification-methodology-aim-tool I don't think this is being updated anymore. There is also an internal version that contains CBI that the PMN folks use, which contains a lot more data. If you want access to the CBI version of AIM, just ask Gino Scarano about it. I am not sure if it needs to be added to your VDI access or not. As for a threshold, there are two search criteria, called pass 1 (more stringent) and pass 2 (less stringent). Pass 1 selects analogues when all of the fragments, atoms, etc., are present, but neither option provides a percent similarity or anything like that. Also, I think some of the PMN folks probably use the analogue search functionalities in OECD Toolbox, ChemID, and/or PubChem, but I am not sure.

Todd

TODD J. STEDEFORD, PH.D., DABT®, ERT, ATS®
OF COUNSEL
BERGESON & CAMPBELL PC
2200 Pennsylvania Avenue, NW, Suite 100W | Washington, D.C. 20037
T: 202-557-3833 | F: 202-557-3836 | lawbc.com

From: Jarabek, Annie <Jarabek.Annie@epa.gov>
Sent: Wednesday, August 18, 2021 12:34 PM
To: Todd J. Stedeford, Ph.D., DABT®, ERT, ATS <TStedeford@lawbc.com>
Subject: [EXTERNAL] Can you tell me

Hi Todd

Hope you are still happy as a clam in your new workplace. I am relieved or perhaps blissfully unaware of any future developments…

Can you tell me the name of the software for read across that PMN program uses? Is there a threshold for determining sufficiently similar?

I am gradually digging out from my backlog and will be pressing to do the corrective MPPD simulations soon on PSLT and GS.

Annie